An Approximation Theorist's View on

Solving Operator Equations

- with special attention to Trefftz, MFS, MPS, and DRM methods -

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Abstract: When an Approximation Theorist looks at well-posed PDE problems or operator equations, and standard solution algorithms like Finite Elements, Rayleigh-Ritz or Trefftz techniques, methods of fundamental or particular solutions and their combinations, they boil down to approximation problems and stability issues. These two can be handled by Approximation Theory, and this paper shows how, with special applications to the aforementioned algorithms. The intention is that the Approximation Theorist's viewpoint is helpful fur readers who are somewhat away from that subject.

1 Introduction

Whenever a specific unknown function u^* is to be numerically constructed from whatever known information $D(u^*)$ about it, an Approximation Theorist will first look at *trial spaces* that can approximate the function well, including its data. Whatever the potential numerical recipes are, the resulting errors for the calculated trial functions \tilde{u} should always be comparable to the achievable error when approximating the true solution directly from the trial space, because that error cannot be improved.

To make this argument work, operator equations and numerical algorithms come in the way, unfortunately, and need to be surpassed, but they are not directly relevant to the Approximation Theorist's argument. Consequently, this viewpoint does not really care for the PDE or operator equation problem, and rightfully so, because it turns out that convergence rates are not PDE-dependent, if *stability* can be guaranteed. Then they depend only on the obtainable approximation error, and the latter depends on the true solution, its smoothness, and the chosen trial space. The PDE problem does not matter, as long as stability prevails, in a sense to be worked out.

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1 INTRODUCTION

Consequently, an Approximation Theorist will use solution techniques that are approximation problems as well, and then the error analysis turns out to be quite simple, as will be shown. The basic obstacles are stability problems that will be handled via well–posedness of the operator equations, but then convergence rates can be played back to Approximation Theory, as expected.

This paper approaches these goals step by step, summarizing results from [33, 34, 35], in a more concise form than before, and applying them later explicitly to Trefftz, MFS, MPS, and DRM cases in specialized sections. Readers may be puzzled by the fact that Approximation Theorists avoid linear systems of equations and prefer to work in terms of spaces, not bases. But it will be clear why. It simplifies things and avoids additional instabilities.

The first step concerns *analytic theory*, starting from a general formulation of *well*posed linear operator equations that allow FEM, Trefftz, MFS, and MPS methods. It is assumed that the analytic problem has a solution, and that the operators themselves are not discretized, i.e. differential and boundary operators are not replaced by finite differences, but applied directly to trial functions. The differential and boundary operators that are defining a PDE problem are merged into one single data map $D : U \to F$ that maps a function $u \in U$ to the values $D(u) \in F$ of the operators in question. Solving the problem then consists of inverting D. A typical case would be $D(u) = (-\Delta u, u_{|_{\Gamma}})$ for a Poisson problem with Dirichlet data. It will be assumed that the problem is stated in the form D(u) = f for a given $f \in F$, but it is also assumed to be solvable by a function u^* , i.e. $f = D(u^*)$ holds for some $u^* \in U$. Furthermore, the problem should be well-posed in the sense

$$\|u\|_{WP} \le C_{WP} \|D(u)\|_F \text{ for all } u \in U, \tag{1}$$

i.e. each function should be continuously recoverable from its data. The above *well-posedness norm* $\|.\|_{WP}$ should be weaker than the norm $\|.\|_U$ on U and is of central importance to the error analysis to follow. In case of elliptic boundary value problems with the Maximum Principle, the *well-posedness norm* will be the sup norm. This finishes the PDE side. The rest of the argumentation will not depend on the PDE anymore, once the data map, the spaces, their norms, and the true solution are fixed together with a well–posedness inequality (1). We shall illustrate this in Section 2.

The second step is Approximation Theory. One should choose a finite-dimensional trial space $U_r \subset U$ that is able to approximate the true solution u^* well. If it does so, it will also approximate the data $D(u^*) = f$ of u^* well, i.e. one rather considers the approximation of $f = D(u^*)$ by functions $f_r \in F_r := D(U_r) \subset F$ and expects

that Approximation Theory has good news about the obtainable minimal error

$$\inf_{f_r \in F_r} \|f - f_r\|_F = \|f - f_r^*\|_F =: \eta(f, F_r, F).$$
(2)

These approximations will hopefully determine the convergence rate of the algorithms that are to be defined for PDE solving as well, and the rate will hopefully not depend on the PDE problem. The well-known standard example is that the classical FEM convergence rate is the PDE-independent convergence rate of piecewise linear approximations in Sobolev spaces. But this basic PDE-independence of convergence rates holds in general and comes from Approximation Theory. We add details in Section 3.

The third step is *Theoretical Numerical Analysis*. If one solves approximation problems instead of solving linear systems, namely by minimizing the residuals $f - D(u_r) = D(u^*) - D(u_r)$ over all $D(u_r)$ in *F*, the convergence rates of the previous Approximation Theory step carry over to the numerical solution of the PDE problem, and stability is automatically guaranteed by well-posedness. This is easy to see via $F_r := D(U_r)$ and

$$\|u^* - u_r^*\|_{WP} \le C_{WP} \|f - D(u_r^*)\|_F \le C_{WP} \eta(f, F_r, F),$$
(3)

and is quite satisfactory, as far as error analysis and convergence rates are concerned. Stability problems do not arise as long as the analysis uses spaces, not bases. Summarizing:

Theorem 1. Let a problem in the form D(u) = f with a data map $D : U \to F$ be given and assume it is well–posed in the sense of (1). Pick a trial space $U_r \subset U$, form the space $F_r = D(U_r)$ and approximate f from F_r in the norm on V via (2). Then the optimal solution $f_r^* = D(u_r^*)$ satisfies the error bound (3), i.e. the error in the solution, measured in the well–posedness norm, is is proportional to the error of approximating the data of the true solution.

But the previous step employed approximation in *function spaces*, and this is not easy to handle in practice. It concerned a much too theoretical instance of Numerical Analysis. Therefore we have to deal with a fourth step, namely the problem of *Discretization in Approximation Theory*, replacing functions by finitely many values. This has nothing to do with PDE theory again, but it arises in the background of numerical methods like MFS, MPS, Trefftz, or DRM. It is the part of Numerical Analysis that handles approximation problems in function spaces and breaks them down to some form of Linear Algebra or Optimization. Here, stability issues creep in through the back door. It will be proven in Section 4 that certain approximation problems allow uniformly stable discretizations, if functions are replaced by

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sufficiently many values, and this applies to certain well-posed PDE problems or operator equations in strong formulation. The final sections illustrate these results for Trefftz techniques, the Methods of Fundamental or Particular Solutions, and the Dual Reciprocity Method. The experimental paper [31] has many numerical examples that support an Approximation Theorist's view on these methods.

But before we go on, here is a seemingly trivial practical consequence of Theorem 1 concerning an a-posteriori error analysis:

Corollary 1. For a well–posed problem in the above sense, assume that a function $\tilde{u} \in U$ is produced by whatsoever method, and assume that the norm $||f - D(\tilde{u})||_F$ can be calculated. Then

$$\|u^* - \tilde{u}\|_{WP} \le C_{WP} \|f - D(\tilde{u})\|_F$$

is an error bound involving only the well-posedness constant.

Unfortunately, the literature on operator equations only rarely yields explicit upper bounds for C_{WP} . This topic deserves much more attention in mathematical research.

But the above argument allows a fair comparison of different numerical methods that produce numerical solutions \tilde{u} for the same well-posed problem. Even if C_{WP} is not known, it is independent of the numerical techniques, and the actual error $||f - D(\tilde{u})||_F$ of approximating the data is a valuable information for the comparison of methods. Far too many numerical papers insist on knowing the true solution, and produce examples with unrealistically smooth true solutions. Instead, it suffices to reproduce the data in the norm $||.||_F$ well, and hopefully better than competing methods. If the data error $||f - D(\tilde{u})||_F$ is presented in a paper, and if the error does not meet the expectations of Approximation Theory, there is a serious stability flaw in the presented method that needs special attention.

2 Operator Equations

We first specify which operator equations we shall consider, and how standard PDE problems are subsumed.

By Section 1 an Approximation Theorist sees solving operator equations as a numerically motivated detour from the central problem of approximating the true solution u^* by functions from the trial space. The detour is necessary, because one has only indirect information about the solution, e.g. values of derivatives at

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certain places, or values of integrals of derivatives against certain test functions. These are the available *data* $D(u^*)$ of u^* .

Thus an operator equation takes the form

$$D(u) = f \tag{4}$$

for a *data map* $D : U \to F$ between Banach spaces that is to be inverted. In particular, we assume that $f = D(u^*)$ is given, i.e. the problem is exactly solvable by some $u^* \in U$. The data map simply describes what is known about the solution, e.g. the pair $D(u) := ((-\Delta u)_{|\Omega}, u_{|\partial\Omega})$ for a standard strong Poisson problem on a bounded domain Ω .

Besides solvability, we require *well-posedness* of the operator equation in the sense of a *well-posedness inequality* (1). This implies continuous invertibility of D, but needs some explanation, because it concerns the norms in U and F. The norm in F also arises in the approximation problem (2) and should not be too exotic. A typical bad case arises when setting up PDE problems in Hölder or Sobolev space, because these carry norms that are not easy to access numerically.

For classical strong Dirichlet problems for uniformly elliptic self-adjoint secondorder differential operators L on compact domains Ω with boundary Γ , there is a well-posedness inequality [3, p.14]

$$\|u\|_{\infty,\Omega} \le \|u\|_{\infty,\Gamma} + C\|Lu\|_{\infty,\Omega} \text{ for all } u \in U := C^2(\Omega) \times C(\Gamma)$$
(5)

in the sup norm on U. Then we can choose the right-hand side as our norm in U and get well-posedness also in the norm on U. The data space is $F = C(\Omega) \times C(\Gamma)$ and carries manageable norms, the data map being defined via

$$D(u) := (Lu_{|_{\Omega}}, u_{|_{\Gamma}})$$
 for all $u \in U$.

Weak problems are different, because they have other data maps. Authors should always consider strong and weak "formulations" as completely separate problems, not just two aspects of the same thing. The difference comes up when we write the data maps in terms of infinitely many conditions. The strong Poisson problem on Ω has infinitely many equations

$$\begin{array}{rcl} -\Delta u(x) &=& f(x) &=& -\Delta u^*(x), & x \in \Omega, \\ u(y) &=& g(y) &=& u^*(y), & y \in \partial \Omega \end{array} \tag{6}$$

while the corresponding weak problem consists of

$$\begin{array}{rcl} (\nabla u, \nabla v)_{L_2(\Omega)} &=& (v, f)_{L_2(\Omega)} &=& (\nabla u^*, \nabla v)_{L_2(\Omega)}, & v \in H_0^1(\Omega), \\ u(y) &=& g(y) &=& u^*(y), & y \in \partial\Omega, \end{array}$$
(7)

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just another set of infinitely many equations. Note that by mixture of the above cases one can pose very many different problems, with all kinds of differential and boundary operators. But we refer the reader to [34] for details on handling classical local and global weak problems with this approach.

For Trefftz methods [29, 22, 21, 23], one ideally has a homogeneous differential equation and poses only boundary conditions. Then the data map D can consist only of the boundary values, and the space U should be restricted beforehand to homogeneous solutions. The Method of Fundamental Solutions (MFS, [24, 2, 19, 20, 9, 14, 28, 6]) is a special case. Details will be in Section 6.

If the homogeneous problem has a Maximum Principle, the well-posedness follows from it via

$$||u||_{\infty,\Omega} \leq ||u||_{\infty,\Gamma} = ||D(u)||_{\infty,\Gamma}$$
 for all $u \in U$

with the well-posedness norm $\|.\|_{WP} = \|.\|_{\infty,\Omega}$. Trefftz methods for problems without a Maximum Principle need a different way of proving well-posedness.

The Method of Particular Solutions (MPS [1, 38, 8, 7, 13, 25, 4]) will be shown in Section 7 to inherit its well–posedness from the well–posedness of the PDE problem.

3 Approximation Problems

We now forget operator equations until Section 6 and consider approximation problems (2) on data spaces F. These finite-dimensional linear approximation problems clearly have solutions, but we are interested in the error $\eta(f, F_r, F)$ in terms of the arguments. In many cases, Approximation Theory has good and handy results, but other situations may be still open, e.g. the approximation by traces of Fundamental Solutions, see Section 6. In general, errors decrease with trial spaces getting larger and f getting smoother, at certain rates that are found in the literature.

In general, users should try to get as much information on u^* and $f = D(u^*)$ as possible, and then select trial spaces $F_r = D(U_r)$ that approximate $f = D(u^*)$ well. It will be shown below that the attainable approximation error dominates the error in the operator equation solution, if stability issues are handled properly. Remember that, in contrast to standard *h*-type finite elements, the approach from Approximation Theory is free to choose good trial spaces, and this freedom should be used wisely and not be overdone.

For an extreme case, consider papers concerned with solving some PDE problem in 2D, and providing an example with a true solution u^* like

$$u^*(x,y) = \exp(ax + by)$$

for certain constants a and b, or other cases where one takes the exponential function of a low-degree polynomial. There are plenty of such papers, e.g. [17, 18] for two randomly chosen recent instances. The solution can be approximated by a polynomial of low degree to machine precision, the convergence being exponential in terms of the degree, for the function itself and all derivatives. No matter what the PDE problem in the background is, as long as polynomials are taken as trial functions, one has a numerical problem of just a few degrees of freedom, and one should not need many data to get a solution up to very good accuracy, whatever the PDE problem is. If there is no exponential convergence, something has gone wrong. The same holds if the trial functions themselves have very good approximations by polynomials, e.g. multiquadrics. Then one approximates an approximate polynomial by approximate polynomials, and this can only fail if the authors commit certain numerical crimes that we have to consider in what follows. It does not make sense to take trial spaces that are not close to polynomials in such a case, but if non-polynomial trial spaces are used, papers should contain an experimental comparison to polynomials that may outperform the trial space actually used.

4 Discretizing Approximation Problems

We now reconsider approximation problems (2) on data spaces F, but from a numerical perspective. In view of Corollary 1, we want a numerical method that produces a function $\tilde{f}_r \in F_r$ with

$$\|f - \tilde{f}_r\|_F \le C_A \|f - f_r^*\|_F$$
(8)

with a factor $C_A \ge 1$ that should be independent of F_r . If this works, Corollary 1 yields the error bound

$$||u^* - \tilde{u}_r||_{WP} \le C_{WP}C_A||f - f_r^*||_F = C_{WP}C_A\eta(f, F_r, F)$$

for $\tilde{u}_r \in U$ with $D(\tilde{u}_r) = \tilde{f}_r$ in terms of the error provided by Approximation Theory, and we are done.

But the problem with (8) is that one cannot work directly on functions in Numerical Analysis. The standard discretization in Numerical Analysis replaces functions by finitely many of their values, using a surjective *test* or *sampling* map

4 DISCRETIZING APPROXIMATION PROBLEMS

 $T_s : F \to V_s$ that takes each function $f \in F$ into a vector $T_s(f)$ in a value space V_s of finitely many real numbers, e.g. values at points, or integrals against test functions. Of course, there is no stable recovery of f from $T_s(f)$ because we have only finitely many data.

Then (2) is replaced by a *discrete* approximation problem

$$\inf_{f_r \in F_r} \|T_s(f) - T_s(f_r)\|_{V_s} = \|T_s(f) - T_s(f_{r,s}^*)\|_{V_s} =: \eta(T_s(f), T_s(F_r), V_s)$$
(9)

with a solution $f_{r,s}^* \in F_r$ that can actually be calculated up to roundoff effects and numerical instabilities like bad choices of bases. To allow some leeway, one may assume that one actually produces a $\tilde{f}_{r,s} \in F_r$ with

$$||T_s(f) - T_s(\tilde{f}_{r,s})||_{V_s} \le 2\eta(T_s(f), T_s(F_r), V_s).$$
(10)

When writing $\tilde{f}_{r,s} = D(\tilde{u}_{r,s}) \in U_r$ due to $F_r = D(U_r)$, the error bound (3) turns into

$$\|u^* - \tilde{u}_{r,s}\|_{WP} \leq C_{WP} \|f - D(\tilde{u}_{r,s})\|_F$$

but we have no grip on $||f - D(\tilde{u}_{r,s})||_F$. Instead, we have $||T_s(f) - T_s(D(\tilde{u}_{r,s}))||_{V_s}$, but this is only a discrete norm. We need the transition from $||T_s(f)||_{V_s}$ to $||f||_F$, but this can only work on finite-dimensional subspaces.

Fortunately, Approximation Theory [30] helps with this again, because one can ask for a *stability inequality*

$$||f_r||_F \le C_{r,s} ||T_s(f_r)||_{V_s} \text{ for all } f_r \in F_r$$

$$\tag{11}$$

that inverts the sampling on the values of the trial space. This allows to let the transition from the full approximation problem (2) to the discrete problem (9) be stable in the sense

$$\begin{aligned} \|f - f_{r,s}\|_{F} &\leq \|f - f_{r}^{*}\|_{F} + \|f_{r}^{*} - f_{r,s}\|_{F} \\ &\leq \eta(f, F_{r}, F) + C_{r,s}\|T_{s}(f_{r}^{*}) - T_{s}(\tilde{f}_{r,s})\|_{V_{s}} \\ &\leq \eta(f, F_{r}, F) + C_{r,s}\|T_{s}(f_{r}^{*}) - T_{s}(f))\|_{V_{s}} + C_{r,s}\|T_{s}(f) - T_{s}(\tilde{f}_{r,s})\|_{V_{s}} \\ &\leq \eta(f, F_{r}, F) + 3C_{r,s}\eta(T_{s}(f), T_{s}(F_{r}), V_{s}). \end{aligned}$$

Theorem 2. Let a well-posed operator equation D(u) = f in the sense of Section 2 be given, and assume that for a trial space U_r there is a test discretization on F via sampling maps T_s with (11) for $F_r = D(U_r)$. Then the approximate solution $\tilde{f}_{r,s} = D(\tilde{u}_{r,s})$ of the discretized approximation problem (9) with (10) satisfies the error bound

$$\|u^* - \tilde{u}_{r,s}\|_{WP} \le C_{WP}(\eta(f, F_r, F) + 3C_{r,s}\eta(T_s(f), T_s(F_r), V_s))$$
(12)

in terms of approximation errors.

5 STABILITY INEQUALITIES

This boils the problem down to stability inequalities (11) where we hope to bound $C_{r,s}$ independent of r and s. Note that this form of stability is necessary whenever one works on finite values instead of functions and wants to conclude that small discrete errors lead to small errors in function space. The latter cannot be bypassed, because discrete norms will not work in well-posedness inequalities. Any technique that goes down to a finite system of equations or a finite approximation problem will have to cope with such a stability argument, but experience shows that authors only rarely care for the problem. If the data error $||T_s f - T_s D(\tilde{u}_{r,s})||_{V_s}$ in an application paper does not behave like what Approximation Theory predicts for $||f - T_s D(u_r^*)||_F = \eta(f, F_r, F)$, either C_A or $C_{r,s}$ is not kept at bay, i.e. there is a flaw in the algorithm.

5 Stability Inequalities

These are an interesting and important part of Numerical Analysis, and should be brought to the attention of a wider audience. We start with a seemingly simple classical case.

Assume a user wants to work in the space C[-1,+1] with polynomials of order M, i.e. degree M-1. All functions are replaced by their values on a set $X_N := \{x_1, \ldots, x_N\} \subset [-1,+1]$, and to let this identify polynomials of order M properly, one should let X_N consist of $N \ge M$ different points, by the Fundamental Theorem of Algebra. A *stability inequality* like (11) then is

$$||p||_{\infty,[-1,+1]} \leq C_{M,X_N} ||p||_{\infty,X_N}$$

for all polynomials of order M, but what is the minimal stability constant C_{M,X_N} ?

The answers of Approximation Theory are disppointing at first sight:

- 1. For M = N and equidistant points, C_{M,X_N} grows exponentially with M.
- 2. For M = N and Chebyshev-distributed points, C_{M,X_N} grows logarithmically with M.

But if *oversampling* is used, the situation is *much* better:

- 1. For $N \ge \pi M$ and Chebyshev-distributed points, C_{M,X_N} is bounded independent of M.
- 2. For $N \ge CM^2$ and equidistant points, C_{M,X_N} is bounded independent of M.

The upshot is that replacing functions from an M-dimensional trial space by $N \ge M$ function values is unstable unless values are taken at well-chosen points and a serious amount of oversampling is applied. For users solving operator equations, using exotic trial spaces on nontrivial domains, this fact has to be taken into account, because unbounded stability constants $C_{r,s}$ spoil the approximation error rates in (12). The same holds if users insist on having square linear systems. If these arise from discretizing functions, instability *must* be expected. However, if users choose examples with extremely smooth true solutions that lead to very good or even exponential convergence, the effect is not observable.

But a sufficient amount of oversampling can lead to uniform stability under certain circumstances. We state a special case of a result of [34] based on the extremely useful *norming set* notion of [16]:

Theorem 3. For the space $F = C(\Omega)$ of continuous functions on a compact set Ω under the sup norm and all finite-dimensional subspaces F_r there is a set $X_{s(r)}$ of points of Ω such that $C_{r,s(r)} \leq 2$.

A weak variant is

Theorem 4. For the space $F = L_2(\Omega)$ of square-integrable functions on a compact set Ω under the L_2 norm and all finite-dimensional subspaces F_r there is a set of normalized test functionals defining a sampling operator T_s such that $C_{r,s(r)} \leq 2$.

Like in Section 2, the difference between the strong and weak case lies in what *data* means. In Theorem 4, normalized test functionals are L_2 integrals against compactly supported test functions with norm 1.

The above cases apply whenever the data space *F* consists exclusively of parts that behave like $C(\Omega)$ or $L_2(\Omega)$. This fails if well-posedness is stated in Hölder norms, but there is a bypass that will be treated elsewhere.

6 Trefftz Problems

As stated in section 2, a Trefftz problem for a homogeneous differential equation with a Maximum Principle reduces to approximation on $C(\Gamma)$ in the sup norm. Thus Theorem 3 applies to the stability problem, implying

Theorem 5. Assume a well-posed problem for a homogeneous differential equation and Dirichlet boundary values, with the Maximum Principle being satisfied. Then for any trial space of homogeneous solutions there is a sufficiently fine set of test points on the boundary that guarantees uniform stability. \Box

7 METHOD OF PARTICULAR SOLUTIONS

It remains to check the approximation problem (2) in $F = C(\Gamma)$. If played back to a trial space $U_r \subset U$ of homogeneous solutions, it turns into

$$\inf_{u_r \in U_r} \|u^* - u_r\|_{\infty,\Gamma} =: \eta(u^*_{|_{\Gamma}}, U_{r|_{\Gamma}}, C(\Gamma))$$

and now the ball lies in the field of Approximation Theory, but the latter has not much to say about this, unfortunately.

If specialized to the MFS, the classical trial space consists of fundamental solutions centered on a *fictitious boundary* outside of the domain, but the approximation error is measured on the true boundary. This is a nasty approximation problem that should get much more attention by Approximation Theorists. The papers [32, 15] use special kernel-based trial spaces where these approximation errors can be calculated, without any fictitious boundary. For the special case of equidistant points on concentric circles and conformal images of such configurations, results of Katsurada [19, 20], handle the problem nicely by Fourier analysis. However, a good general theory is still missing.

7 Method of Particular Solutions

Here one only has a differential operator as the data map $D : U \to F$, and one works with pairs $(u_j, f_j) = (u_j, D(u_j))$ of trial functions spanning trial spaces U_r and $F_r = D(U_r)$, respectively. Then, given a function $f \in F$, the approximation problem (2) is posed, and this is completely independent of PDEs. If an approximation $\tilde{f}_r \in F_r$ is found, one has a function $\tilde{u}_r \in U_r$ with $D(\tilde{u}_r) = \tilde{f}_r$ that is taken as the desired result.

However, the approximation problem (2) needs a discretization. If carried out in $C(\Omega)$ with the sup norm, we can invoke Theorem 3, implying

Theorem 6. Assume a differential operator $D : C^p(\Omega) \to F = C(\Omega)$ of order p on a compact domain $\Omega \subset \mathbb{R}^d$. Then for any choice (U_r, F_r) of trial spaces of particular solutions with $F_r = D(U_r)$, there is a finite set $X \subset \Omega$ such that the discretized approximation problem in the sup norm on X is uniformly stable in the sense of Section 4, i.e. the full approximation error is at most twice the discrete approximation error.

Often, the choice of the f_j is done first, in order to use results on the approximation error by these functions, but then one has to calculate the u_j in order to transfer the approximation back to U. In other cases, based on the smoothness of u^* , one can use functions u_j that give good approximation errors including higher derivatives, and then the calculation of the f_j is easy.

8 DUAL RECIPROCITY METHOD

To compare these two in the kernel-based situation using the Whittle–Matérn kernels generating Sobolev spaces $W_2^m(\mathbb{R}^d)$, we take the uniformly elliptic differential operator $D = Id - \Delta$ that maps isometrically from $W_2^m(\mathbb{R}^d)$ to $W_2^{m-2}(\mathbb{R}^d)$ and back, by Fourier transform theory. Let us assume that the true solution u^* is in $W_2^m(\mathbb{R}^d)$. If we start from translates of the kernel of $W_2^m(\mathbb{R}^d)$ and form the images under D, we know [36] that the L_∞ error in F behaves like $h^{m-2-d/2}$ where h is the fill distance of the centers used to generate the trial spaces. If we work backwards, we have to approximate $f = D(u^*)$, but this is only in $W_2^{m-2}(\mathbb{R}^d)$, and the best possible approximation error in L_∞ is again of order $h^{m-2-d/2}$. This implies that finding the u_j from the f_j by complicated arguments is likely not to pay off. The error is comparable in both cases. The MPS can be effectively carried out from trial spaces U_r in U, using the spaces $F_r = D(U_r)$ for the approximation of f.

8 Dual Reciprocity Method

But the Method of Particular Solutions ignores boundary conditions. The standard application is a two-step technique for a problem of the form D = (L, B) with a differential operator *L* and a boundary operator *B*, called *Dual Reciprocity Method* [26, 27, 5].

If the problem is posed as $D(u) = (L(u), B(u)) = f = (f_L, f_B)$, the MPS is applied first to come up with an approximate solution of $L(u) = f_L$, i.e. with a function u_{MPS} such that

$$||f_L - L(u_{MPS})||_F \leq \varepsilon_{MPS}$$

The previous section dealt with this part, including stability and error bounds.

The second step takes the boundary values of u_{MPS} and solves the homogeneous problem Lu = 0 with $B(u) = f_B - B(u_{MPS})$ by a Trefftz or MFS technique. If we stabilize the approximation on the boundary along the lines of Section 6, we get

$$\|B(\hat{u}) - B(\tilde{u})\|_{\infty,\Gamma} \leq \varepsilon_T$$

for the approximate solution \tilde{u} and the true solution \hat{u} for the above homogeneous problem.

Note that both steps did not assume a full well-posedness. If we now assume a well-posed Dirichlet problem with the Maximum Principle in the sense of (5), our previous arguments imply

$$\begin{aligned} \|u^* - \tilde{u} - u_{MPS}\|_{\infty,\Omega} &\leq \|u^* - \tilde{u} - u_{MPS}\|_{\infty,\Gamma} + \|L(u^* - \tilde{u} - u_{MPS})\|_{\infty,\Omega} \\ &= \|B(\hat{u}) - B(\tilde{u})\|_{\infty,\Gamma} + \|f_L - L(u_{MPS})\|_{\infty,\Omega} \\ &\leq \varepsilon_T + \varepsilon_{MPS}. \end{aligned}$$

9 Direct Optimal Recovery

We viewed methods for solving operator equations as an approximation of a function u^* from their data $D(u^*)$. In section 2 we looked at well-posed problems where u^* is fully and stably determined by the full data $D(u^*)$ comprising infinitely many conditions, like in (6) and (7). Later, in Section 4, we went back to only partial and finite data in order to have a numerically manageable problem.

From an Approximation Theory viewpoint, this can be seen as a detour. If only finitely many data $\lambda_1(u^*), \ldots, \lambda_M(u^*)$ for linear functionals $\lambda_1, \ldots, \lambda_M \in U^*$ are given right from the beginning, e.g. a finite selection of the data functionals in (6) or (7), we should find the best approximation to u^* using this information only.

Of course, this needs some regularization, and a simple way [37] is to go into a suitable Hilbert space $H \subseteq U$ on which the functionals are continuous and to construct the function $\tilde{u} \in H$ that has smallest norm and shares the same data, i.e. satisfies the generalized interpolation conditions $\lambda_j(u^*) = \lambda_j(\tilde{u}), 1 \leq j \leq M$. By standard arguments, the solution is a unique linear combination of the representer functions u_1, \ldots, u_M in H of the functionals $\lambda_1, \ldots, \lambda_M$, the coefficients being obtainable by solving a positive definite Gramian matrix with entries $(\lambda_j, \lambda_k), 1 \leq j, k \leq M$.

By another standard argument, the value $\tilde{u}(x)$ for any fixed x is the best linear prediction of any function value there, provided that only the given data are available. Given H and the data, there is no better way of solving the problem pointwise. From a Machine Learning viewpoint in Hilbert Spaces, this is an optimal way of learning the solution of an operator equation from given training data.

However, the method is not new at all. In the context of kernel-based techniques, it is Symmetric Collocation [37, 10, 12, 11, 35], but it can also be seen as a Rayleigh-Ritz method. Due to its optimality properties, it is impossible to be outperformed error–wise for the given data, but is has serious stability and complexity drawbacks that are hard to overcome. A special case, connected to Trefftz methods and confined to potential problems, is in [32, 15], but it deserves extensions using new kernels implementing singularity-free homogeneous solutions of other differential operators.

References

[1] K.E. Atkinson. The numerical evaluation of particular solutions for Poisson's equation. *IMA Journal of Numerical Analysis*, 5:319–338, 1985.

- [2] A. Bogomolny. Fundamental solutions method for elliptic boundary value problems. *SIAM J. Numer. Anal.*, 22:644–669, 1985.
- [3] D. Braess. *Finite Elements. Theory, Fast Solvers and Applications in Solid Mechanics*. Cambridge University Press, 2001. Second edition.
- [4] C. S. Chen, C. M. Fan, and P. H. Wen. The method of approximate particular solutions for solving certain partial differential equations. *Numer. Methods Partial Differential Equations*, 28(2):506–522, 2012.
- [5] C.S. Chen, C.A. Brebbia, and H. Power. Dual reciprocity method using compactly supported radial basis functions. *Comm. Num. Meth. Eng.*, 15:137– 150, 1999.
- [6] C.S. Chen, A. Karageorghis, and Y.S. Smyrlis. *The Method of Fundamental Solutions - A Meshless Method*. Dynamic Publishers, 2008.
- [7] C.S. Chen, A.S. Muleshkov, and M.A. Golberg. The numerical evaluation of particular solution for Poisson's equation - a revisit. In C.A. Brebbia and H. Power, editors, *Boundary Elements XXI*, pages 313–322. WIT Press, 1999.
- [8] C.S. Chen and Y.F. Rashed. Evaluation of thin plate spline based particular solutions for Helmholtz-type operators for the DRM. *Mech. Res. Comm.*, 25:195–201, 1998.
- [9] G Fairweather and A. Karageorghis. The method of fundamental solution for elliptic boundary value problems. *Advances in Computatonal Mathematics*, 9:69–95, 1998.
- [10] G. Fasshauer. Solving partial differential equations by collocation with radial basis functions. In A. LeMéhauté, C. Rabut, and L.L. Schumaker, editors, *Surface Fitting and Multiresolution Methods*, pages 131–138. Vanderbilt University Press, Nashville, TN, 1997.
- [11] C. Franke and R. Schaback. Convergence order estimates of meshless collocation methods using radial basis functions. *Advances in Computational Mathematics*, 8:381–399, 1998.
- [12] C. Franke and R. Schaback. Solving partial differential equations by collocation using radial basis functions. *Appl. Math. Comp.*, 93:73–82, 1998.
- [13] M.A. Golberg. Recent developments in the numerical evaluation of particular solutions in the boundary element method. *Appl. Math. Comp.*, 75:91– 101, 1996.

- [14] M.A. Golberg and C.S. Chen. The method of fundamental solutions for potential, Helmholtz and diffusion problems. In M.A. Golberg, editor, *Boundary Integral Methods: Numerical and Mathematical Aspects*, pages 103– 176. WIT Press, 1998.
- [15] Y.C. Hon and R. Schaback. Solving the 3D Laplace equation by meshless collocation via harmonic kernels. *Adv. in Comp. Math.*, pages 1–19, 2013.
- [16] K. Jetter, J. Stöckler, and J.D. Ward. Error estimates for scattered data interpolation on spheres. *Mathematics of Computation*, 68:733–747, 1999.
- [17] E. Kansa. Radial basis functions: achievements and challenges. In A.H. Cheng and C. Brebbia, editors, *Boundary Elements and Other Mesh Reduction Methods XXXVII*, volume 61, pages 3–22. WIT Transactions on Modelling and Simulation, 2015.
- [18] A. Karageorghis, M. Jankowska, and C.S. Chen. Kansa-RBF algorithms for elliptic problems in regular polygonal domains. *Numerical Algorithms*, pages 1–23, Dec. 2017.
- [19] M. Katsurada. Asymptotic error analysis of the charge simulation method in a jordan region with an analytic boundary. *Journal of the Faculty of Science of Tokyo University, Section 1A*, 37:635–657, 1990.
- [20] M. Katsurada. Charge simulation method using exterior mapping functions. *Japan Journal of Industrial and Applied Mathematics*, 11:47–61, 1994.
- [21] J.A. Kolodziej and A.P. Zielinski. *Boundary Collocation Techniques and their Application in Engineering*. WIT Press, 2009.
- [22] Z.-C. Li, T.-T. Lu, H.-Y. Hu, and A. H.-D. Cheng. *Trefftz and collocation methods*. WIT Press, Southampton, 2008.
- [23] Z.C. Li, L.J. Young, H.T. Huang, and A.H.-D. Liu, Y.P. Cheng. Comparisons of fundamental solutions and particular solutions for Trefftz methods. *Eng. Anal. Bound. Elem.*, 34(3):248–258, 2010.
- [24] R. Mathon and R.L. Johnston. The approximate solution of elliptic boundary-value problems by fundamental solutions. *SIAM J. Numer. Anal.*, 14:638–650, 1977.
- [25] A.S. Muleshkov, C.S. Chen, M.A. Golberg, and A.H-D. Cheng. Analytic particular solutions for inhomogeneous Helmholtz-type equations. In S.N. Atluri and F.W. Brust, editors, *Advances in Computational Engineering & Sciences*, pages 27–32. Tech Science Press, 2000.

- [26] D. Nardini and C.A. Brebbia. A new approach to free vibration analysis using boundary elements. In C.A. Brebbia, editor, *Boundary Element Methods* in Engineering, Proc. 4th Int. Sem., pages 312–326. Springer-Verlag, 1982.
- [27] P.W. Partridge, C.A. Brebbia, and L.C. Wrobel. *The Dual Reciprocity Boundary Element Method*. CMP/Elsevier, 1992.
- [28] A. Poullikkas, A. Karageorghis, and G. Georgiou. The method of fundamental solutions for inhomogeneous elliptic problems. *Computational Mechanics*, 22:100–107, 1998.
- [29] Q.-H. Qin. *The Trefftz Finite and Boundary Element Method*. WIT Press, 2000.
- [30] C. Rieger, B. Zwicknagl, and R. Schaback. Sampling and stability. In M. Dæhlen, M.S. Floater, T. Lyche, J.-L. Merrien, K. Mørken, and L.L. Schumaker, editors, *Mathematical Methods for Curves and Surfaces*, volume 5862 of *Lecture Notes in Computer Science*, pages 347–369, 2010.
- [31] R. Schaback. An adaptive numerical solution of MFS systems. In C.S. Chen, A. Karageorghis, and Y.S. Smyrlis, editors, *The Method of Fundamental Solutions - A Meshless Method*, pages 1–27. Dynamic Publishers, 2008.
- [32] R. Schaback. Solving the Laplace equation by meshless collocation using harmonic kernels. *Adv. in Comp. Math.*, 31:457–470, 2009. DOI 10.1007/s10444-008-9078-3.
- [33] R. Schaback. Unsymmetric meshless methods for operator equations. *Numerische Mathematik*, 114:629–651, 2010.
- [34] R. Schaback. All well–posed problems have uniformly stable and convergent discretizations. *Numerische Mathematik*, 132:597–630, 2015.
- [35] R. Schaback. A computational tool for comparing all linear PDE solvers. *Advances of Computational Mathematics*, 41:333–355, 2015.
- [36] H. Wendland. *Scattered Data Approximation*. Cambridge University Press, 2005.
- [37] Z. Wu. Hermite–Birkhoff interpolation of scattered data by radial basis functions. *Approximation Theory and its Applications*, 8/2:1–10, 1992.
- [38] S. Zhu. Particular solutions associated with the Helmholtz operator used in DRBEM. *Boundary Element Abstracts*, 4:231–233, 1993.